Int J Life Cycle Assess (2008) 13:328–338
DOI 10.1007/s11367-008-0004-1

WOOD AND OTHER RENEWABLE RESOURCES • CASE STUDY

Wax production from renewable feedstock using biocatalysts instead of fossil feedstock and conventional methods

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Received: 1 December 2006 / Accepted: 21 February 2008 / Published online: 17 May 2008

Abstract
Background, aim, and scope Using renewable feedstock and introducing biocatalysts in the chemical industry have been suggested as the key strategies to reduce the environmental impact of chemicals. The Swedish interdisciplinary research program "Speciality Chemicals from Renewable Resources—Greenchem" is aiming to develop these strategies. One target group of chemicals for Greenchem are wax esters which can be used in wood coatings to replace paraffin wax made from fossil crude oil. The aim of this study was to conduct a life cycle assessment of wax esters based on rapeseed oil produced by biocatalysts (enzymes). The scope was to compare the environmental performance of wax esters with paraffin wax produced by conventional methods.
Materials and methods The study has a cradle-to-gate perspective and the functional unit is "1-kg wax product ready to use in a wood coating product." Extensive data collection and calculations have been performed for the wax esters, whereas existing life cycle inventory data have been used for the paraffin wax.
Results The energy input into the wax ester production is about one third of the energy input in paraffin wax production. However, the wax ester has a higher contribution to the global warming potential (GWP) due to high emissions of nitrous oxide from rapeseed cultivation. Referring to a cradle-to-grave perspective, including waste incineration, the contribution to the GWP will, however, be 3.5 times higher from paraffin wax. Wax ester makes a higher contribution to the acidification and eutrophication potential, due to emissions from soil from rapeseed cultivation, but five times lower contribution to the photochemical ozone creation potential. From a land-use perspective and a global warming point of view, it is more efficient to produce paraffin wax and grow high-yielding, short-rotation coppice (Salix) to replace fuel oil than it is to grow rapeseed for wax ester production.
Discussion Overall, this study shows the importance of studying the environmental performance of a product not only from a gate-to-gate perspective but, instead, considering the environmental performance from cradle-to-gate. The biocatalytic production of the wax ester consumes less energy than the conventional chemical method, but the raw material step, cultivation of rapeseed contributes much to both acidification and eutrophication. When the waste treatment step is included, the contribution to GWP, however, for paraffin wax will be 3.5 times higher than for the wax ester.
Conclusions From a gate-to-gate perspective, replacing conventional chemical processes by biocatalysts using enzymes leads to energy savings and reduces emissions. However, from a cradle-to-gate perspective, the use of renewable feedstock, such as rapeseed oil, may counteract some of these benefits. Concerning the GWP benefit from using renewable feedstock instead of fossil feedstock, the final waste treatment step must be included, thereby applying a cradle-to-grave perspective.
Recommendations and perspectives The introduction of biocatalysts as a key strategy in reducing the environmental impact from the chemical industry is supported by the results in this study. On the other hand, it is not obvious that the key strategy of using renewable feedstock in chemical production per se leads to benefits concerning all environmental impact categories. Thus, much more attention

Responsible editor: Jörg Schweinle

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needs to be paid to the choice of potential renewable feedstock options, the minimization of energy inputs, and the biological emissions from the soil in the cultivation of feedstock crops, improved gas cleaning in nitrogen fertilizer production plants, and the alternative use of the arable land, in optimizing the overall environmental benefits of an increased use of renewable feedstock in the chemical industry.

Keywords Biocatalyst · Fossil feedstock · Greenchem · Land use · Life cycle assessment (LCA) · Rapeseed oil · Renewable raw material · Wax ester · Wood and other renewable resources

1 Background, aim, and scope

An increased use of renewable feedstock and biotechnological processes within the chemical industry are often suggested as key strategies in achieving a more resource—and environmentally—sustainable industrial production. The chemical industry has become increasingly dependent on fossil feedstock as the raw material for both bulk and fine chemicals. Besides being a limited resource, the combustion of fossil feedstocks contributes to the greenhouse effect. Petroleum-based products are often degraded slowly or not at all when released into the environment, leading to problems in waste management. Establishing "clean" process technologies that would decrease the consumption of energy and nonrenewable raw materials and reduce or eliminate waste is, thus, a key to prevent pollution at source. Alternative synthetic pathways using alternative solvents require improved and selective catalysis which has a potential to reduce the number of stages in a given process and, hence, reduce its environmental impact. Because spent catalysts at the end of a reaction also constitute chemical waste, their recycling is also necessary. These factors favor the use of biocatalysts (enzymes) which are selective and do not involve toxic metals that are normally present in chemical catalysts. They are also naturally adapted to processing renewable feedstocks.

The research program "Speciality Chemicals from Renewable Resources—Greenchem" is a Swedish interdisciplinary research program which focuses on the development and application of biocatalysts for the production of fine chemical products from renewable raw materials. The programme includes research activities both within biotechnology and environmental systems analysis and cooperates with several industrial partners from raw material producers to end-use industry. One target group of chemicals in the Greenchem program is wax esters based on vegetable oil (rapeseed oil) and produced by biocatalysts, following the 12 principles of Green Chemistry (Anastas and Warner 1998). The biotechnological method using biocatalysts (enzymes) for producing behenyl behenate is a process that is not widely commercialized today and is under development within the Greenchem program. This wax ester can be used to replace paraffin wax produced from crude oil in several kinds of applications, for example, not only within the pharmaceutical and health-care industry but also in various wood coatings. Efforts have been made finding life cycle assessments (LCAs) on other similar products. This, however, turned out to be hard. The only available study found was Thum and Oxenbøll (2006), where the industrial biocatalytic production of myristyl myristate at Degussa was studied. In this study, the production of the raw material is not included, but the results are similar as for the biocatalytic production step in our study, showing large savings in energy and emissions of unwanted pollutants.

The purpose of our paper is to compare the environmental performance of a wax ester, behenyl behenate ($C_{44}H_{88}O_2$) with ordinary paraffin wax produced from fossil oil. The analysis includes the life cycle from cradle to gate of the two products. Another aim is to identify the steps in the life cycle which give rise to the most significant environmental impact (hot spots) and to suggest improvements in the systems studied. Attention will also be paid to the impact of alternative land-use strategies for biomass production and greenhouse gas reduction.

2 Materials and methods

The life cycle assessment performed in this paper follows the methodology standardized in ISO 14040-43 (1998). The systems investigated, including cradle-to-gate, were divided into several subsystems, shown in Fig. 1. In the calculations, all transport is taken into account. Focus in this article is the production of behenyl behenate. Therefore, each individual step in the production procedure is investigated. Paraffin wax is used here as a reference case. Here, existing life cycle inventory (LCI) data have been used, which are presented only in an aggregated form.

2.1 Functional unit

The functional unit is the definition of the functional outputs of the product system, and the functional unit in a life cycle assessment provides a reference to which the inputs and outputs can be related. For this study, the functional unit is defined as*: 1-kg wax product ready to use in a wood coating product*, with wax product here meaning either wax ester or paraffin wax. The products investigated can be used in the same way and with the same amount within a final wood coating product.

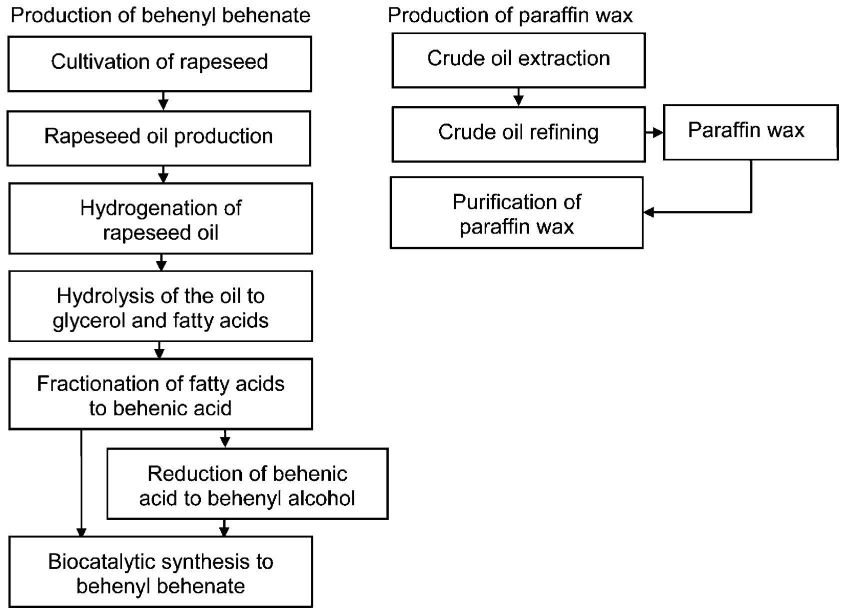

Fig. 1 Flow-chart showing the subsystems included for production of behenyl behenate and for the reference case, production of paraffin wax

2.2 The calculations—assumptions and input data

Data on rapeseed cultivation and rapeseed oil production are based on Bernesson (2004), whereas data of wax ester production are based on our own calculations together with data from Bernesson (2004) and Karlshamns AB (Petersson 2005). The inventory data used for the calculations for paraffin wax was collected from Boustead (2003). These data have also been complemented with data received from Akzo Nobel Industrial Coatings AB (Lindell 2005).

In Bernesson (2004), other available data on rapeseed production was studied and, thus, cross-checked. The values obtained by Gärtner and Reinhardt (2001) and Reinhardt and Gärtner (2002) conducted under German and Central European conditions, for example, were very similar to the ones used by Bernesson, the results for most impact categories differed by less than 20% (Bernesson 2004).

The production of the wax ester is assumed to take place in Sweden using Swedish average electricity (Uppenberg et al. 2001a, b). In the study, calculations using primary energy have been used. Efforts have been made using the most recent data available in literature.

Crude oil is a mixture of hydrocarbons of molecules containing from three to many hundred carbon atoms. LCI data for the production of paraffin wax from crude oil are based on Boustead (2003). The environmental impact from the production of 1-kg paraffin wax has been estimated to be equivalent to the environmental impact of the production of 2 kg of naphtha (Lindell 2005; Hauschild et al. 2003). The LCI data for paraffin wax are based on average data from several different sources. For both behenyl behenate and paraffin wax, fuel-cycle emissions and primary energy have been included in the calculations.

2.3 Allocation

When a production process generates several products, the total environmental load of the system has to be shared among these different products by allocation. Different methods may be used for allocation in LCA, for instance, physical or economic allocation. In this analysis, physical allocation has been utilized, which is based on the mass of each product. The LCI data from the literature used in this analysis are based on physical allocation. Examples of allocations made are in the refining of crude oil where paraffin wax and other petroleum products are produced and in rapeseed oil production where meal is produced as a by-product to be used as fodder. However, LCI data found for rapeseed oil production also include economic allocation between the rapeseed oil and meal. This allocation method is tested in the sensitivity analysis.

One way to avoid allocation is to use system expansion. In this case, the rape meal produced in the process could, e.g., replace imported soy meal. This was conducted in Bernesson (2004) as a sensitivity analysis, together with an extensive analysis of the effects of choosing different allocation methods. For a further discussion of the influence of different systems boundaries and allocation methods, see Bernesson (2004).

2.4 Impact categories

The impact assessment methodology in this study follows the customer minutes lost 2001. The emissions to air included in the LCA are: carbon dioxide (CO_2, fossil origin), carbon monoxide (CO), hydrocarbons (HC, except methane), methane (CH_4), nitrogen oxides (NO_x), sulfur

oxides (SO_x), ammonia (NH_3), nitrous oxide (N_2O) and hydrochloric acid (HCl). Emissions to water include nitrate (NO_3^-). The environmental indicator and impact categories chosen are global warming potential (GWP), acidification potential (AP), eutrophication potential (EP), photochemical oxidant creation potential (POCP), and energy consumption. The category indicators are presented in Table 1.

3 System description—production of behenyl behenate

3.1 Cultivation of rapeseed

The cultivation of high erucic rapeseed was assumed to be located in the flatlands of Svealand in Central Sweden. The harvest was assumed to be 2,470 kg rapeseed per hectare, containing 8% water and 45% oil (wet weight basis; Bernesson 2004). The emissions from soil of ammonia were calculated to be 40 g NH_3/kg fertilizer nitrogen, and nitrous oxide emissions 19.6 g N_2O/kg fertilizer nitrogen applied, which was calculated to amount to 140 kg N ha^{-1} $year^{-1}$(Bernesson 2004; Jungk et al. 2000). The LCI data on rapeseed cultivation have been complemented with emissions of NO_3^- to water here calculated to be 133 kg NO_3^- ha^{-1} $year^{-1}$ (Jungk et al. 2000; Johnsson and Mårtensson 2002).

Nitric acid is used in the manufacturing in commercial nitrogen fertilizers, such as ammonium nitrate, calcium nitrate, and potassium nitrate. The main atmospheric emissions from the production of nitric acid are N_2O and NO_x. The amount of N_2O emitted per kilogram nitrogen produced in commercial fertilizers used in rapeseed cultivation is estimated to be, on average, 18.6 g based on current average data from fertilizer production plants in Western Europe (Davis and Haglund 1999). For more specific information about the cultivation of rapeseed, see Bernesson (2004).

3.2 Production of rapeseed oil

The extraction of rapeseed oil was assumed to be done in a strainer type of oil expeller in a large scale plant, assumed to serve an area of 50,000 ha (Bernesson 2004). In large-scale plants, extraction takes place in two steps, pressing and hexane extraction, where the oil extraction efficiency was assumed to be 98%. The energy consumption was 220 MJ electricity/tonne rapeseed or 490 MJ electricity/tonne rapeseed oil.

3.3 Hydrogenation of double bonds in rapeseed oil

The hydrogenation of the double bonds in the rapeseed oil is done with hydrogen and a catalyst, usually a precious metal, often platinum. The reaction takes place under high pressure and high temperature. Approximately 70 Nm^3 hydrogen is needed per tonne fatty acid ester (Petersson 2005). To produce this hydrogen, electrolysis is used and the energy consumption is 1,480 MJ/tonne (50% electricity and 50% steam) fatty acid ester.

For all the chemical steps described here, namely, the hydrogenation of double bonds, the hydrolysis of oil to fatty acids, the fraction of fatty acid to behenic acid, the reduction of behenic acid to behenyl alcohol and, finally, the biocatalytic synthesis to behenyl behenate, 50% of the energy consumed come from electricity and 50% from steam. The steam is to 25% from liquefied petroleum gas and 75% is produced with woodchips, based on average Swedish conditions (Petersson 2005).

3.4 Hydrolysis of the oil to glycerol and fatty acids

For the hydrolysis of rapeseed oil to rapeseed fatty acid, 560 MJ of energy (50% electricity and 50% steam) is needed per tonne (Petersson 2005). A by-product in this hydrolysis is glycerol.

Table 1 Category indicators used in the study

Emissions to air	**$GWP_{100\ years}$ g CO_2 eq/g**	**AP g SO_2 eq/g**	**EP g PO_4^{3-} eq/g**	**POCP g C_2H_4 eq/g**
CO_2	1	–	–	–
SO_x	–	1	–	–
NO_x	–	0.7	0.13	–
NH_3	–	1.88	0.35	–
CO	2	–	–	0.04
CH_4	23	–	–	0.007
HC		–	–	0.4
N_2O	296	–	–	–
HCl	–	0.88	–	–
Emissions to water				
NO_3^-	–	–	0.10	–

High erucic rapeseed contains about 45% C22 which is used for the production of behenic acid. It is here assumed that 1 tonne high erucic rapeseed gives 400 kg erucic acid, which is hydrated to behenic acid. The rest of the rapeseed ends up as other fatty acids (C16–C20), glycerol, and pitch. A yield of more than 100% may be received depending on the water generated during the hydrolysis (Petersson 2005).

3.5 Fractionation of fatty acids to behenic acid

To produce clean behenic acid, the hydrogenated product also needs fractionated distillation. Total energy consumption (50% electricity and 50% steam) for this step is set to 3,000 MJ/tonne, from triglyceride from erucic acid to 1,000 kg ready-to-use, distilled behenic acid and approximately 80 kg distilled glycerol (by-product). If upgrading of the glycerol is excluded, the net energy consumption is about 2,320 MJ/tonne, the figure used in the calculations (Petersson 2005).

3.6 Reduction of behenic acid to behenyl alcohol

To produce the behenyl alcohol needed to produce behenyl behenate, the behenic acid must be reduced. The energy requirement for this step has been assumed based on experience from similar processes. The energy requirement was assumed to be 1,110 MJ/tonne (50% electricity and 50% steam). No specific data were found for the reduction step of behenic acid to behenic alcohol; therefore, the energy demand for this step had to be based on one's own assumptions.

3.7 Biocatalytic synthesis to behenyl behenate

The energy demand for the biocatalytic synthesis is here set to 1,110 MJ/tonne (50% electricity and 50% steam), based on average data calculated from six potential production systems. The biocatalytic synthesis to behenyl behenate can be done using two different reactor systems, either a batch or a continuous reactor. Calculations for a large-scale plant for the production of behenyl behenate were conducted. The calculations for the production facility were done for six different reactor systems, using air-stripping or evaporation for water removal. The reactor was heated by circulating hot water in a mantle around the reactor and/or by preheating the air used for water removal. Both batch and continuously stirred tank reactors were evaluated. The calculations were based on reactor volumes suitable for an annual production of 50 tonnes, which was estimated to be two 102-l reactors for the batch system and one 22-l reactor for the continuous system. For the reactor, 20 mm of insulation was used, and a heat exchanger with an efficiency of 83% was assumed for in- and outgoing air flows where applicable. The efficiency of the air heating was assumed to be 90%. For detailed information on the biocatalytic production of behenyl behenate, see Petersson et al. (2005). The production of the enzyme (Novozyme 435) is not included in this study.

4 Results

The results for the two waxes evaluated are shown in Figs. 2 and 3. The production of the wax ester based on rapeseed has a greater environmental impact than paraffin wax for all categories except POCP. In all categories, it is the cultivation of rapeseed that has the largest environmental impact. The emissions of nitrous oxide (N_2O) from the cultivation and rapeseed oil production step represent more than 70% of the total impact affecting global warming. These emissions come to 50% from production and use of fertilizers and to 50% from soil emissions. In the sensitivity analysis, variations in N_2O emissions from soil are tested.

Because behenyl behenate is based on a renewable resource and paraffin wax is not, this will significantly affect the contribution to the global warming when the disposal stage is also included. Because the two products are assumed to be used as an ingredient in a wood coating, it can be assumed that the coatings will be incinerated after use. Thus, Fig. 2 also shows the GWP for the two waxes including the waste incineration stage. Based on this cradle-to-grave perspective, the contribution to the GWP will be 3.5 times higher from paraffin wax than from behenyl behenate.

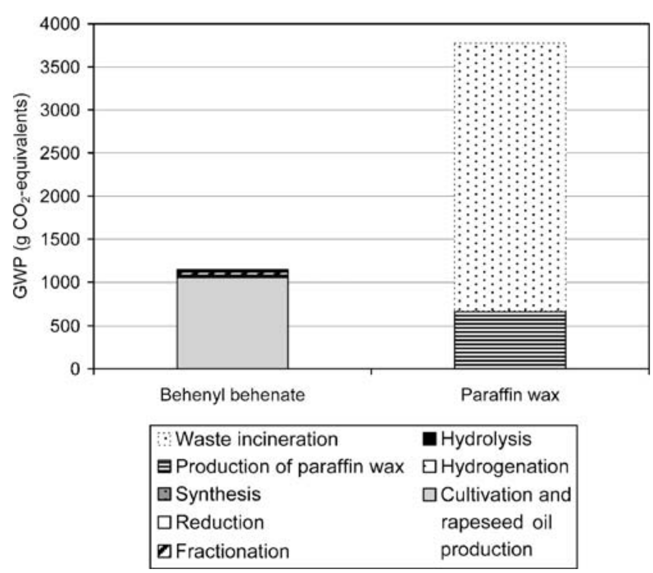

Fig. 2 The contribution to the global warming potential (GWP) per functional unit from the production of behenyl behenate and paraffin wax. The contribution to the GWP from cradle-to-grave, including waste incineration, is also shown

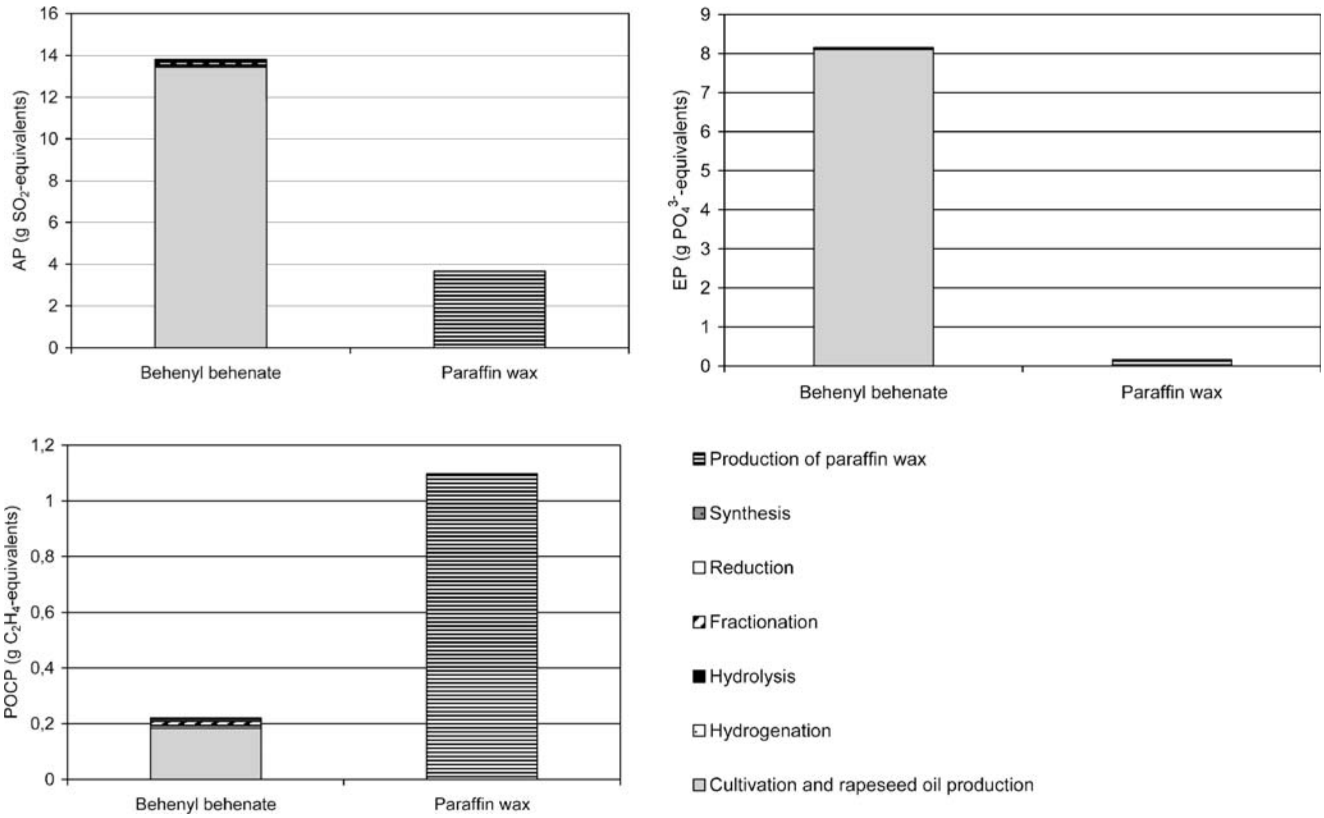

Fig. 3 The contribution to the acidification potential (*AP*), eutrophication potential (*EP*) and the photochemical ozone creation potential (*POCP*) per functional unit from the production of behenyl behenate and paraffin wax

The incineration of the paraffin wax, and of the behenyl behenat, will cause other emissions affecting other impact categories as well. An estimation in this analysis, however, is that these emissions will be almost similar for the two products and also nearly insignificant from a life cycle perspective. Thus, the effects of the disposal stage are here focusing on the difference between the products and only on the effects of significant importance.

The results in Fig. 3 show that behenyl behenate makes a contribution to both AP and EP that is several times larger than the contribution from paraffin wax, 14 g SO_2 equivalents compared to 3.7 g SO_2 equivalents per functional unit and 8.2 g PO_4^{3-} equivalents compared with 0.17 g PO_4^{3-} equivalents per functional unit. The step including cultivation of rapeseed and the rapeseed oil production affects both acidification and eutrophication the most, more than 90% of the contribution to AP and EP from behenyl behenate comes from this phase. The large contributions are due to the leakage of nitrogen during cultivation.

Paraffin wax contributes to the POCP almost five times as much as behenyl behenate, 1.1 g C_2H_4 equivalents compared to 0.23 g C_2H_4 equivalents per functional unit for behenyl behenate. The result for POCP is shown in Fig. 3. The big contribution from paraffin wax comes from large emissions to air of hydrocarbons.

The energy demand for the two products is shown in Table 2. The green wax ester, behenyl behenate, has an energy demand that is only one third of the energy demand for paraffin wax, 28.1 MJ/kg behenyl behenate compared to 101 MJ/kg paraffin wax. Paraffin wax has an energy demand of 101 MJ/functional unit (Boustead 2003).

Table 2 Energy demand per functional unit for the different production steps for behenyl behenate

Production step	Energy demand (MJ) Behenyl behenate
Cultivation of rapeseed	18.9
Rapeseed oil production	2.75
Hydrogenation	1.48
Hydrolysis	0.56
Fractionation	2.32
Reduction	1.11
Synthesis	1.11
Total	**28.2**

4.1 Sensitivity analysis

In Fig. 4, the sensitivity of using economic instead of physical allocation, as in the base-case, is shown for rapeseed cultivation and rapeseed oil production. The meal produced in the process is used as fodder, which has a lower economical value, about 20% of the value of rapeseed oil. The environmental impact from the cultivation of rapeseed and rapeseed oil production will, then, be shared 75.5% vs. 24.5% between oil and fodder instead of 45% vs. 55% on the physical allocation. The contribution to the GWP of behenyl behenate will increase by almost 65% from 1150 g CO_2 equivalents to 1,900 g CO_2 equivalents per functional unit. Because the changes are similar for all impact categories, we have chosen only to show the changes for GWP.

The emissions from the soil from cultivation may vary significantly due to local conditions. Here, the emissions of N_2O are assumed to be equivalent to 1.25% kg^{-1} added nitrogen, which is also the current recommended factor by Intergovernmental Panel on Climate Change to use in greenhouse gas inventories (IPCC 1996). According to other studies, the biological N_2O emissions originating from fertilizers may vary from almost 0% to 2%, or even 3% (Jungk et al. 2000; Nevison et al. 1996). Based on new results from an extensive amount of field trial measurements, the N_2O factor is recommended to be reduced equivalent to 0.8% kg^{-1} nitrogen fertilizer supplied, concerning ammonium nitrate fertilizers (Bouwman et al. 2002a, b). A decrease in N_2O emissions equivalent to 0.5% of the nitrogen supplied will reduce the GWP for behenyl behenate from 1,150 g CO_2 equivalents to 935 CO_2 equivalents per functional unit, a decrease by 18%. An increase equivalent to 2%, on the other hand, will increase the GWP from 1150 g CO_2 equivalents to 1,350 g CO_2 equivalents per functional unit, an increase by 18%, see Fig. 5.

4.1.1 Emissions during cultivation

The emission of N_2O from the production of nitrogen fertilizers has been estimated to vary between 15 and 21 g N_2O kg^{-1} nitrogen in Swedish fertilizer production,

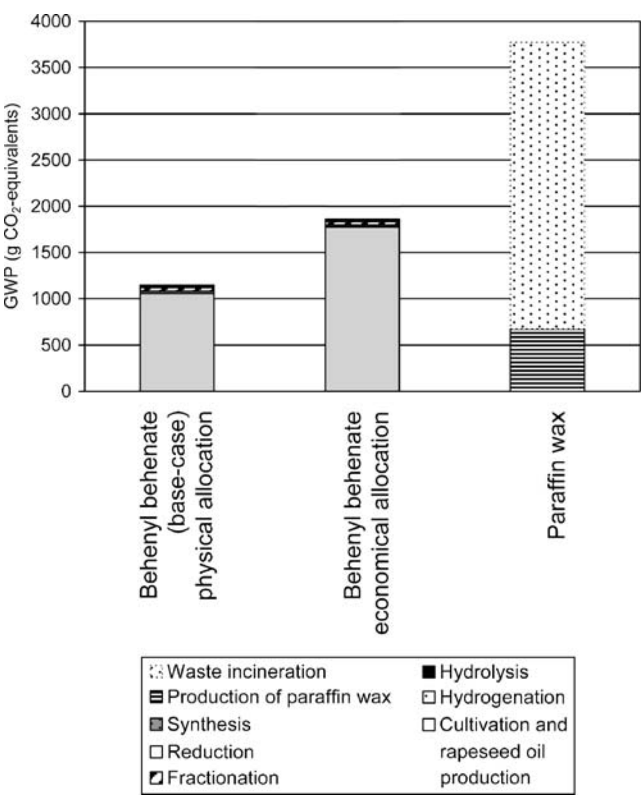

Fig. 4 Changes in the cultivation to the GWP per functional unit from the production of behenyl behenate when economical allocation for cultivation of rapeseed and production of rapeseed oil is used instead of physical allocation (base-case)

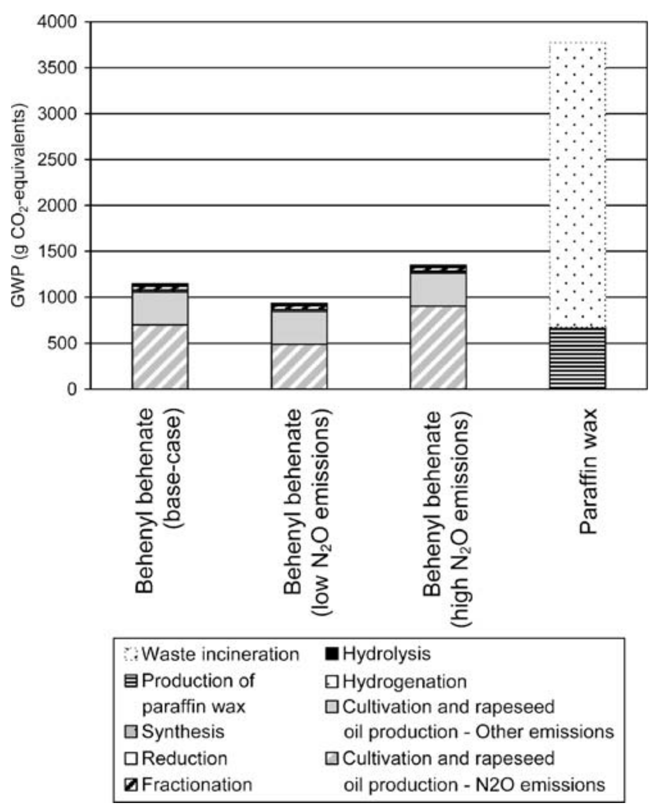

Fig. 5 Changes in the contribution to the GWP per functional unit from the production of behenyl behenate when the soil emissions of nitrous oxide (N_2O) is reduced (low N_2O emissions equivalent to 0.5% of the nitrogen fertilizer supplied), or increased (high N_2O emissions equivalent to 2%), compared with the base-case (N_2O emissions equivalent to 1.25% of the nitrogen fertilizer supplied)

depending on type of fertilizer (excluding urea) and production plant (Davis and Haglund 1999). Average data from fertilizer production in Western Europe show a variation between 11 and 30 g N_2O kg^{-1} nitrogen, depending on the type of commercial nitrogen fertilizer produced (excluding urea; Davis and Haglund 1999). Thus, compared with the average data used in this paper (18.6 g N_2O kg^{-1} nitrogen), this potential variation in emission of N_2O in fertilizer production (±40 to 60%) is somewhat lower than the estimated potential variation in the biological emissions of N_2O from the soil. However, the emissions of N_2O from the nitrogen fertilizer production plants may be significantly reduced by improved cleaning technology, e.g., by installing catalytic gas cleaning. This development is already on its way, why the emission of N_2O from the production of nitric acid is estimated to be significantly reduced in a near future. Thus, the contribution to the GWP from the cultivation of rapeseed will, then, also be reduced.

The amount of commercial nitrogen fertilizer supplied during the rapeseed cultivation will have a significant environmental impact. One reason is due to the emission of N_2O during the production of the nitrogen fertilizers, and one other reason is the potential biological emission of fertilizer-induced N_2O from the soil. In this study, the amount of nitrogen fertilizer supplied during the rapeseed cultivation is estimated, on average, to be 140 kg nitrogen per ha. Based on current practical fertilization recommendations in Sweden, the application ration of nitrogen fertilizer may vary from about 100 up to 200 kg/ha, depending on the geographical location of cultivation, the fertility of the soil, and whether winter rape or spring rape is cultivated. Expressed per amount of rapeseed harvested, however, the variation in nitrogen fertilizer supplied is rather small.

The potential nutrient leaching from arable land depends on various factors, such as cropping systems, fertilization strategies, precipitation, and soil type. Rapeseed cultivation is here estimated to cause nitrogen leaching equivalent to 30 kg N ha^{-1} $year^{-1}$, based on average conditions in Central and Southern Sweden. However, the leakage from rapeseed cultivation within these regions may vary from about 10 to 70 kg N ha^{-1} $year^{-1}$ depending on local conditions (Johnsson and Mårtensson 2002). In Fig. 6, the sensitivity of a change in nitrogen leaching (equivalent to 15 and 45 kg ha^{-1} $year^{-1}$) on the EP is shown. A decrease in nitrogen leaching from 30 to 15 kg ha^{-1} $year^{-1}$ will reduce the EP for behenyl behenate from 8.6 g PO_4^{3-} equivalents to 5.7 g PO_4^{3-} equivalents per functional unit, a decrease by 33%. An increase equivalent to 45 kg ha^{-1} $year^{-1}$ will increase the EP by 33% to 12 g PO_4^{2-} equivalents per functional unit. Even with the low nitrogen leaching equivalent to 15 kg N per ha, the contribution to EP from behenyl behenate is more than 20 times greater than the contribution from paraffin wax.

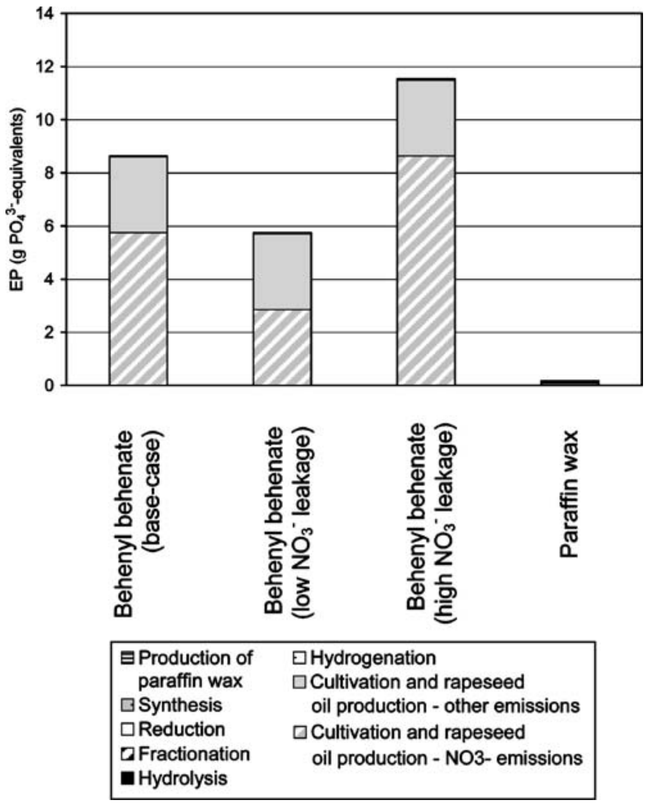

Fig. 6 Changes in the contribution to the EP per functional unit from the production of behenyl behenate when the nitrogen leaching is reduced (low NO_3^- leaching equivalent to 15 kg N ha^{-1} $year^{-1}$), or increased (high NO_3^- leaching equivalent to 45 kg N ha^{-1} yr^{-1}), compared with the base-case (NO_3^- leaching equivalent to 30 kg N ha^{-1} yr^{-1})

4.1.2 Land use

Another important aspect when doing life cycle assessments on products based on biomass produced on agriculture land is the alternative use of the land needed. This aspect has often been overlooked in previous LCA studies of biomass-based chemical products (Dornburg et al. 2004). Perhaps the land utilized for cultivation of rapeseed can be used more efficiently in, for instance, reducing greenhouse gases. This aspect is considered here and includes two alternatives of land use to the base-case. In the base-case, it is assumed that if the land is not used for cultivation of rapeseed, it would lie in follow. A comparison was conducted in which the cultivation of rapeseed was carried out, using all the by-products (straw, meal, and glycerol) for energy recovery, replacing heating oil. Another case will assume the land to be used for growing short-rotation coppice (Salix) for energy production, also replacing heating oil. The harvest of Salix was assumed to be nine dry tonnes, giving an annual energy harvest of 170 GJ/ha (Westin et al. 2003). If all by-products from the cultivation of rapeseed and from rapeseed oil production are used for energy production, an annual energy

harvest of 68 GJ/ha will be achieved (see also Table 3). The greenhouse gas (GHG) emission reductions are shown in Fig. 7. The result shows that the largest saving in GHG emissions is when the land is used for growing energy forest and paraffin wax is produced.

5 Discussion

LCA is often used to reveal the most hazardous steps in the life cycle of a product and to decide which of various alternative products is associated with the least potential impact on the environment. According to OECD (1998), LCA is the best method for determining the increased degree of cleanliness that can be achieved by introducing biotechnological processes. In this study, it is shown, when producing chemicals from rapeseed oil the first step, that cultivation and production of rapeseed oil is the step in the life cycle that has the largest environmental impact. This is the case for all the impact categories studied. When studying only a cradle-to-gate perspective and not including waste handling, the wax ester, behenyl behenate, contributes almost twice as much to global warming than paraffin wax, despite a much lower energy input. This also shows the importance of studying the final step, the waste incineration, because it is here that the difference in GWP between a renewable and nonrenewable feedstock is really shown.

The step, cultivation, and production of rapeseed oil has a significant impact, not only on the GWP but also on acidification and eutrophication, with almost all the contribution to these two categories coming from this step. A suggestion to lower the emissions from this step is to improve fertilizer production to find new ways to fertilize crops or to find a more nutrient efficient method of cultivation. This is the most important finding in this paper, the need of reducing the environmental impact from the raw material production step, in this case the cultivation and production of rapeseed oil. One example is reduced emissions of N_2O from the production of nitrogen fertilizers by installing catalytic gas cleaning in nitric acid production plants, which is an ongoing development today.

Table 3 Energy values for by-products from cultivation of rapeseed and rapeseed oil production (Bernesson 2004)

Type of product	kg/ha	MJ/kg	GJ/ha
Rapeseed oil	1,090	38.3	41.7
Meal	1,330	15.3	20.4
Straw	3,210	14.1	45.2
Glycerine	115	17.1	1.97
Total			**109**

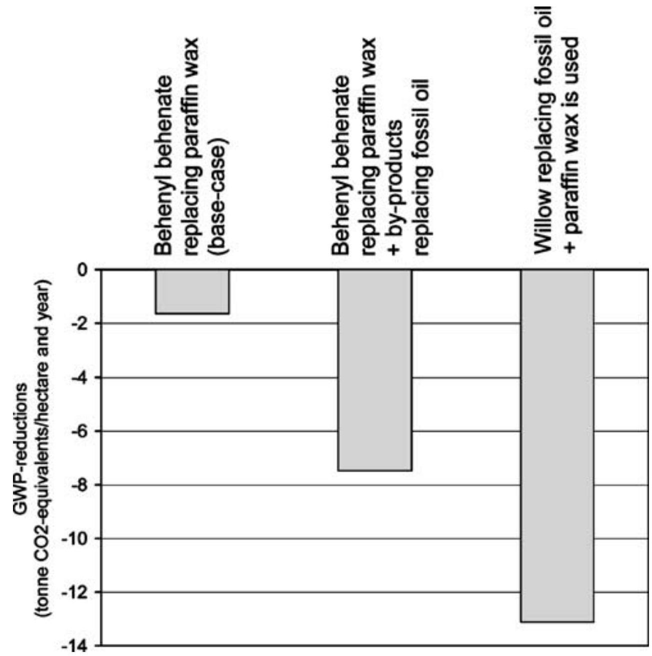

Fig. 7 The reduced contribution to the GWP per hectare and year when behenyl behenate replace paraffin wax (base-case), when also all by-products from the cultivation of rapeseed and rapeseed oil production is used to replace fuel oil, and when short-rotation coppice (willow) is cultivated instead of rapeseed and used to replace fuel oil and paraffin wax is used instead of behenyl behenate

Another alternative to reduce the environmental impact could be to use a different type of vegetable oil. The environmental performance of vegetable oil may differ significantly due to their origin and vegetable oil crop utilized. However, the natural sources of behenic acid are very limited; the only other widely commercial crop containing useable amounts of behenic acid is peanut oil with a content of approximately 3% (Hasenhuettl 2005). Because the wax ester in this study should be used in a wood coating product, different technical specifications have to be fulfilled. One is the melting point that has to be high enough. Therefore, another type of wax ester could not be used in our case (containing a shorter carbon chain). Wax esters, however, are also widely used as ingredients in cosmetic products and to decrease the environmental impact from these products, another type of wax ester based on other vegetable oils might be possible to use. In addition, using biocatalysts instead of using conventional processes will further improve the environmental performance of these products (Thum and Oxenbøll 2006; Petersson 2005).

In the sensitivity analysis, the importance of choosing an accurate allocation method is shown. In the base-case, physical allocation was used to divide the emissions from rapeseed oil production between rapeseed oil and the by-product, rape meal. The results show that by changing to

economic allocation, which in this case could be argued to be more accurate, the environmental impact on global warming from behenyl behenate increases by almost 65%.

In the sensitivity analysis, the importance of making accurate assumptions is also shown. In the first case, the local variations in biological soil emissions have been taken into consideration. The N_2O emissions from the nitrogen fertilizer applied may vary from 0.5–2%, changing the impact of behenyl behenate on global warming with ±18%. In the second case, the variation in nutrient leaching is shown. Here, in the base-case, the leaching of nitrogen per hectare and year is set to 30 kg, but the leaching may vary from 10–70 kg due to local conditions. An increase or decrease in nitrogen leakage by ±50% gives a variation by ±33% for the eutrophication potential. The land-use aspect is sometimes neglected in life cycle assessments, but the results in this LCA show the importance of taking the use of land into consideration. The result, from a global warming perspective, shows that it is better to produce paraffin wax and use the land for growing high-yielding, short-rotation energy forest than it is to grow rapeseed for behenyl behenate production, if one wants to optimize the GHG savings. However, when excluding the land-use aspect, the production of behenyl behenate is a better alternative than producing paraffin wax, from a GHG point of view. This analysis, as well as some other studies (Dornburg et al. 2004), only includes two specific aspects of land use, the potential energy savings and the greenhouse gas emission reductions of biobased products and bioenergy. There are, however, several other aspects related to land use, such as soil erosion, hydrology effects, soil structure, biodiversity and aesthetic value of the landscape (Mattson et al. 2000). These aspects are difficult to quantify and include in life cycle assessments, but there is an ongoing development of methods within this field today.

Utilization of natural, renewable resources in the production of environmentally benign chemicals as substitutes for petroleum-based chemicals has attracted considerable attention during the past decade. Although some examples of biodegradable products, like biodegradable polymers, are being reported, turning from petroleum-based to renewable raw materials is a major challenge. To reduce the number of stages in a given process, and thereby reduce the environmental impact, improved and more selective catalysis is needed. These favor the use of biocatalysts (enzymes) which are selective and do not involve toxic metals that are normally present in chemical catalysts. The biocatalytic process using enzymes to produce behenyl behenate studied here has an energy demand that is 34% lower than the conventional process using high pressure and high temperature. Less waste is also created during the biocatalytic process (Petersson et al. 2005). Despite a number of biocatalyst-based industrial processes (e.g., for the manufacture of aspartame and acryl amide), further efforts are needed in order to make biocatalysts attractive as tools for the chemical industry.

6 Conclusions

Relatively recently, LCA has been recognized as a tool for process evaluation as well, e.g., process optimization (Azapagic 2002). Such LCA studies often exclude the production of the raw material and the use and product disposal stages and, thus, covering only a “gate-to-gate” perspective. The results in this study confirm the environmental benefits from using biocatalysis, although it also shows the importance of including all stages in the life cycle to gain an accurate and comparable result. From a cradle-to-gate perspective, the use of renewable feedstock, such as rapeseed oil instead of fossil feedstock, may counteract some of the benefits from using enzymes instead of conventional processes. In some cases, a change of feedstock, e.g., a vegetable oil crop with lower environmental impact, could be one way to improve the environmental performance of the product. This option, however, is not always possible because different technical specifications must be fulfilled. In this case regarding behenyl behenat, rapeseed oil is the only realistic feedstock alternative due to its favorable composition of fatty acids. A way to reduce the environmental impact of rapeseed production is to improve fertilizer production, to find new ways to fertilize the rapeseed crop, and to find a more nutrient efficient method of cultivation. Concerning the GWP benefit from using renewable feedstock instead of fossil feedstock, the final waste treatment step must be included, thereby applying a cradle-to-grave perspective when doing LCAs.

7 Recommendations and perspectives

Although LCA was developed during the 1970s, it has so far had little impact on the biotechnical product and process sectors (OECD 1998). According to OECD (1998), there are two main reasons why biotechnology is underrepresented in LCAs. The first is the relatively recent appearance of biotechnological processes compared to chemical ones. Only in exceptional cases is sufficient information available on mass and energy flows. The second is the greater methodological difficulty involved in assessing the production of renewable raw materials such as biomass. For example, when renewable materials are used, this raises questions about land-use alternatives and CO_2 credits. Within the Swedish interdisciplinary program, Greenchem, focus is on the development and application of clean processes based on biotechnology for the production of fine chemicals from

renewable raw material. The program includes research activities both within biotechnology and environmental system analysis and cooperates with several industrial partners. Thus, this concept is one way to increase the availability of LCI data and make possible an expansion of LCA in Green Chemistry.

As this study has shown, the introduction of biocatalysts as a key strategy to improve the environmental performance in the chemical industry is a good way to go. On the other hand, it is not obvious that the key strategy of using renewable feedstock in chemical production per se leads to benefits concerning all environmental impact categories. Thus, much more attention needs to be paid to the choice of potentially renewable feedstock options, the minimization of energy inputs and the biological emissions from the soil in the cultivation of feedstock crops, improved gas cleaning in nitrogen fertilizer production plants, and the alternative use of the arable land in optimizing the overall environmental benefits of an increased use of renewable feedstock in the chemical industry. Therefore, LCAs must be used to answer whether a product is environmentally benign or not.

Acknowledgements This study is a part of the research program Greenchem at Lund University, and we gratefully acknowledge the economic support provided by The Foundation for Strategic Environmental Research (MISTRA). Akzo Nobel Industrial Coatings AB (Malmö, Sweden) and Karlshamns AB (Karlshamn, Sweden) are greatly acknowledged for their help with LCI data. We also thankfully acknowledge the advice generously given to us by the wax ester project group at the Department of Biotechnology, Lund University.

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